

Statistical Theory of Finite Fermi-Systems Based on the Structure of Chaotic Eigenstates

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(February 1, 2008)

The approach is developed for the description of isolated Fermi-systems with finite number of particles, such as complex atoms, nuclei, atomic clusters etc. It is based on statistical properties of chaotic excited states which are formed by the interaction between particles. New type of “microcanonical” partition function is introduced and expressed in terms of the average shape of eigenstates $F(E_k, E)$ where E is the total energy of the system. This partition function plays the same role as the canonical expression $\exp(-E^{(i)}/T)$ for open systems in thermal bath. The approach allows to calculate mean values and non-diagonal matrix elements of different operators. In particular, the following problems have been considered: distribution of occupation numbers and its relevance to the canonical and Fermi-Dirac distributions; criteria of equilibrium and thermalization; thermodynamical equation of state and the meaning of temperature, entropy and heat capacity, increase of effective temperature due to the interaction. The problems of spreading widths and shape of the eigenstates are also studied.

I. INTRODUCTION

As is known, quantum statistical laws are derived for systems with infinite number of particles, or for systems in a heat bath, therefore, their applicability to isolated finite systems of a few particles is, at least, questionable. However, the density of many-particle energy levels increases extremely fast (typically, exponentially) both with an increase of number of particles and excitation energy. For this reason, even a weak interaction between particles can lead to a strong mixing between large number of simple many-particle states, resulting in the so-called *chaotic eigenstates*. If the components of such eigenstates can be treated as random variables (onset of *Quantum Chaos*), statistical methods are expected to be valid even for an isolated dynamical system.

One should stress that statistical description of such isolated systems can be quite different from that based on standard canonical distributions; therefore, application of the famous Fermi-Dirac or Bose-Einstein formulae may give incorrect results. Moreover, for isolated few-particle systems a serious problem arises in the definition of temperature, or other thermodynamic variables like entropy and specific heat (to compare with, in infinite systems different definitions give the same result).

The aim of this paper is to develop statistical theory for finite quantum systems of interacting particles, based on generic statistical properties of chaotic eigenstates (“microcanonical” approach). Typical examples of such systems are compound nuclei, complex atoms, atomic clusters, isolated quantum dots, etc.

The structure of the paper is as follows. In the next Section 2, new type of “microcanonical” partition function is introduced for finite isolated systems, which is directly related to the average shape of chaotic eigenstates. Based on this partition function, general expression for the occupation numbers is given which is valid for any number of interacting particles. Relation of this

“microcanonical” expression (F – distribution) to that of standard canonical distribution for occupation numbers is the subject of the Section 3. Also, here a new form of the canonical distribution is suggested which can be convenient in applications to open systems in thermal equilibrium like quantum dots.

Transition to the standard Fermi-Dirac distribution for large systems is analyzed in Section 4. Specific attention is paid to the accuracy of this distribution in applications to isolated systems with few particles.

In Section 5 the analytical derivation of the F –distribution for occupation numbers is given. For this, the model of n randomly interacting Fermi-particles distributed over m single-particle levels has been used. The analytical formula for the occupation numbers $n_s(E)$ with E being the total energy of the system, was found to be in excellent agreement with the numerical experiment.

In Section 6 the influence of finite width of single-particles states (“quasi-particles”) on the distribution of occupation numbers is considered. New expression for the occupation numbers is discussed which takes into account the finite spreading width of “quasi-particles”. It is demonstrated that for an isolated system with the fixed total energy E , the incorporation of spreading widths decreases the effective temperature, however, does not change the occupation numbers.

Section 7 deals with an important problem of thermodynamical description of small systems consisting of finite number of interacting particles. Specifically, different definitions of both temperature and entropy have been analyzed, and the equation of state for finite systems has been derived.

In Section 8 we show that statistical effects of the interaction can be imitated by an increase of the effective temperature. This fact allows to use the standard Fermi-Dirac expression for the occupation numbers (with renormalized parameters) in the application to both isolated and open (in the thermal bath) systems of interacting Fermi-particles. This interaction may be strong, how-

ever, the assumption of randomness for residual interaction matrix elements is essential.

In Section 9 the conditions for chaos, equilibrium and “thermalization” have been analyzed for an isolated quantum system of a finite number of particles in terms of the interaction strength, number of particles and other related parameters. Depending on these conditions, there are four different regions with different distributions of occupation numbers, which are discussed in detail. In this Section, the transition to mesoscopic systems is shortly discussed. The question of particular interest is how statistical properties depend on the dimensionality of a system.

Since the approach developed in this paper is entirely related to the structure of chaotic eigenstates, in Appendix 1 the analytical expression for the average shape of eigenstates is given and discussed in more details. This expression, which also describes the local spectral density of states (LDOS), essentially depends on two different widths and is valid both for weak and strong interaction between particles. For weak interaction the shape is close to the Lorentzian form with the half-width given by the Fermi Golden Rule. For larger interaction the shape is characterized by exponential tails and by the width which is linear in the interaction strength (contrary to the Fermi Golden Rule which gives a quadratic dependence). Transition between these two regimes occurs when the half-width is comparable to the root-mean-square width (effective band width of the Hamiltonian matrix).

In Appendix 2 the moments of the distributions of the basis components (LDOS) and energy levels are calculated.

And finally, in Appendix 3 the calculation of density of final states and spreading widths of the LDOS has been performed using the Fermi Golden Rule.

II. MICROCANONICAL PARTITION FUNCTION

In this Section we are going to derive the partition function for closed (isolated) systems of finite number of interacting particles. This function allows one to perform analytical and numerical calculations of statistical mean values of different operators, for example, occupation numbers.

We follow the standard approach which is based on the separation of a total Hamiltonian in two parts,

$$H = H_0 + V = \sum \epsilon_s a_s^\dagger a_s + \frac{1}{2} \sum V_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \quad (1)$$

The “unperturbed” Hamiltonian H_0 should incorporate the effect of a mean field (if any), ϵ_s are the energies of single-particle states (“orbitals”) calculated in this field, a_s^\dagger, a_s are creation-annihilation operators, and V stands for the residual interaction. For simplicity, here we neglect any dynamical effects of the interaction like pairing, collective modes etc. Instead, we will study statistical effects of interaction, therefore, in what follows we assume

that matrix elements V_{pqrs} of the two-body residual interaction are random variables.

Exact (“compound”) eigenstates $|i\rangle$ of the Hamiltonian H can be expressed in terms of simple “shell-model basis states” $|k\rangle$ (eigenstates of H_0) :

$$|i\rangle = \sum_k C_k^{(i)} |k\rangle ; \quad |k\rangle = a_{k_1}^\dagger \dots a_{k_n}^\dagger |0\rangle \quad (2)$$

These compound eigenstates $|i\rangle$, characterized by the corresponding energies $E^{(i)}$, are formed by the residual interaction V ; in complex systems they typically contain large number $N_{pc} \gg 1$ of the so-called principal components $C_k^{(i)}$ which fluctuate “randomly” as a function of indices i and k .

Our main interest is in the occupation numbers n_s of single-particle states (orbitals). They can be represented in terms of components of the exact eigenstates $|i\rangle$,

$$n_s = \langle i | \hat{n}_s | i \rangle = \sum_k \left| C_k^{(i)} \right|^2 \langle k | \hat{n}_s | k \rangle \quad (3)$$

Here $\hat{n}_s = a_s^\dagger a_s$ is the occupation number operator. The knowledge of the distribution of occupation numbers gives the possibility to calculate mean values of any single particle operator $\langle M \rangle = \sum_s n_s M_{ss}$. Moreover, the variance of the distribution of non-diagonal elements of M describing transition amplitudes between “chaotic” compound states, can be also expressed through the occupation numbers n_s [1,2,3].

As one can see from (3), mean values of occupation numbers depend on the shape of exact eigenstates, given by the “spreading function” F (in what follows, the F – function),

$$F_k^{(i)} \equiv \left| C_k^{(i)} \right|^2 = F(E_k - E^{(i)}) \quad (4)$$

Last equality in the above expression reflects the fact that residual interaction V mainly mixes close components k in some energy interval Γ (“spreading width”) nearby the eigenstate energy $E^{(i)}$ (more accurately, nearby the unperturbed energy E_k for $k = i$, see below).

Typically, this spreading function rapidly decreases with an increase of $|E_k - E^{(i)}|$ (since an admixture of distant component is very small). Recently, in numerical studies of the Ce atom [2], the $s - d$ nuclear shell model [4] and random two-body interaction model [3,5] it was found that typical shape F of exact eigenstates practically does not depend on a particular many-body system and has a universal form which essentially depends on the spreading width Γ . The latter can be expressed in terms of parameters of the model (intensity V of the residual interaction, number of particles n , excitation energy, etc.) and can be calculated analytically (see Appendices 1- 3). One can also measure the width of the F –function (4) via the number of principal components, $N_{pc} \sim \Gamma/D$ where D is the local mean energy spacing

for compound states. In many-body systems the value of D exponentially decreases with an increase of the number of “active” (valence) particles. As a result, N_{pc} is very large, $\sim 10^4 \div 10^6$ in excited (compound) nuclei and ~ 100 in excited rare-earth or actinide atoms.

The starting point of our approach is the expression for the occupation numbers which stems from Eqs. (3,4),

$$n_s(E) = \frac{\sum_k n_s^{(k)} F(E_k - E)}{\sum_k F(E_k - E)} \quad (5)$$

where $n_s^{(k)} \equiv \langle k | \hat{n}_s | k \rangle$ equal 0 or 1 for Fermi-particles and the sum in the denominator stands for the normalization. This way of averaging of occupation numbers is a kind of microcanonical averaging since it is defined for the fixed total energy E of a system. One can see that, in fact, the relation (5) is equivalent to the introduction of a new kind of partition function,

$$Z(E) = \sum_k F(E_k - E) \quad (6)$$

which is entirely determined by the shape of chaotic eigenfunctions. In what follows, we term Eq.(5) the F -distribution.

The above expression (5) gives a new insight on the problem of statistical description of complex systems. Indeed, as was mentioned above, the shape of the F -function has universal features and can be often described analytically, therefore, in practice there is no need to diagonalize huge Hamiltonian matrix of many-body system in order to find statistical averages. One should stress that the summation in (5) is carried out over unperturbed energies E_k defined by the mean field, rather than over the energies of exact eigenstates in the standard canonical distribution. As a result, the distribution of occupation numbers can be derived analytically (see Section 5) even for few interacting particles, in the situation when the standard Fermi-Dirac distribution is not valid.

III. TRANSITION TO THE CANONICAL DISTRIBUTION

It is instructive to compare our F -distribution (5) with occupation numbers obtained by making use of the standard canonical distribution,

$$n_s(T) = \frac{\sum_i n_s^{(i)} \exp(-E^{(i)}/T)}{\sum_i \exp(-E^{(i)}/T)} \quad (7)$$

where T is the temperature and the index i stands for exact eigenstates. The important difference between the F -distribution (5) and the canonical distribution (7) is that in Eq. (5) the occupation numbers are calculated

for a specific energy E of a system unlike specific temperature T in Eq.(7). However, results of calculations based on Eqs. (7) and (5) can be compared with each other using the relation between the energy E and the temperature T ,

$$E = \langle E \rangle_T = \frac{\sum_i E^{(i)} \exp(-E^{(i)}/T)}{\sum_i \exp(-E^{(i)}/T)} \quad (8)$$

The comparison of Eqs. (7) and (5) also shows that the canonical distribution corresponds to the averaging of the “microcanonical” F -distribution over some energy interval Δ_T . To demonstrate this, let us substitute $n_s^{(i)}$ and $|C_k^{(i)}|^2$ from Eqs.(3,4) into Eq.(7) and replace the summation over i by the integration over $\rho(E^{(i)})dE^{(i)}$ where $\rho(E^{(i)})$ is the density of exact energy levels,

$$\sum_i n_s^{(i)} \exp(-E^{(i)}/T) \approx \int n_s^{(i)} \Phi_T(E^{(i)}) dE^{(i)} \quad (9)$$

Here we have introduced the “canonical (thermal) averaging” function,

$$\Phi_T(E) = \rho(E) \exp(-E/T) \quad (10)$$

which is discussed below. As a result, we can transform canonical distribution (7) into the form similar to the F -distribution (5),

$$n_s(T) = \frac{\sum_k n_s^{(k)} F(T, E_k)}{\sum_k F(T, E_k)} \quad (11)$$

where the function $F(T, E_k)$ is the canonical average of $F_k^{(i)}$,

$$F(T, E_k) = \int F_k^{(i)} \Phi_T(E^{(i)}) dE^{(i)} \quad (12)$$

Note that this form of the canonical distribution can be convenient for the calculation of the occupation numbers and other mean values in quantum dots which are in thermal equilibrium with an environment (with no particle exchange).

In large many-body systems the canonical averaging function $\Phi_T(E)$ has narrow maximum since the density of states $\rho(E^{(i)})$ typically grows very fast. The position E_m of its maximum is defined by the expression

$$\frac{d \ln \rho(E)}{dE} = \frac{1}{T} \quad (13)$$

and the width is given by

$$\Delta_T = \left| \frac{d^2 \ln \rho(E)}{dE^2} \right|^{-1/2} \quad (14)$$

As an example, let us consider the system of n interacting particles distributed over m orbitals. In the papers [6,7] it was shown that in the case $m \gg n \gg 1$ the density of states is of the Gaussian form,

$$\rho(E) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(E - E_c)^2}{2\sigma^2}\right) \quad (15)$$

where E_c is the center of the spectrum and σ^2 is its variance. According to recent numerical data [5,3], the Gaussian form for the density $\rho(E)$ occurs also for few particles ($n \geq 4$). This fact allows easily to find the form of $\Phi_T(E)$ which appears to be of quite generic,

$$\Phi_T(E) \sim \exp\left(-\frac{(E - E_m)^2}{2\sigma^2}\right) \quad (16)$$

where

$$E_m = E_c - \frac{\sigma^2}{T} \quad (17)$$

One can see that the width Δ_T of the thermal averaging function equals to the root-mean-square (r.m.s.) width of the spectrum, $\Delta_T = \sigma$. Now, it is easy to show that the thermal averaging width Δ_T is always bigger than the r.m.s. width ΔE of the “microcanonical” F -function or, the same, than the mean width of exact eigenstates in the energy representation. Indeed, there is a simple relation between the widths σ and σ_0 of the energy spectrum with and without interaction, respectively, (see Appendix 1),

$$\sigma^2 = \sigma_0^2 + (\Delta E)^2, \quad (18)$$

therefore, we have $\Delta_T = \sigma > \Delta E$. One should stress that the latter width ΔE , in fact, is due to statistical effects of interaction. The difference between the widths Δ_T and ΔE is not important when the number of particles n is large. This is because with an increase of n the width σ_0 of the unperturbed spectrum increases as \sqrt{n} , unlike the width ΔE which increases as n . One should also note that in this case both widths Δ_T and ΔE are much smaller than the typical energy interval, $\sigma/|E - E_c| \sim 1/\sqrt{n}$. Therefore, for large number of particles the function Φ_T can be regarded as the delta-function at $E = E_m$ and the F -distribution is close to the canonical distribution, see Eq.(12).

To conclude with this Section, the canonical distribution (7) is not correct when describing isolated systems with small number of particles, instead, one should use the F -distribution (5). This was recently confirmed by numerical experiments with the model of few Fermi-particles with two-body random interaction [5,8].

IV. TRANSITION TO THE FERMI-DIRAC DISTRIBUTION

It is instructive now to show how the standard Fermi-Dirac distribution stems directly from the F -distribution (5) in the limit of large number of particles. By

performing explicitly the summation over $n_s = 0$ and $n_s = 1$, the expression (5) can be rewritten in the form

$$n_s(E) = \frac{0 + Z_s(n-1, E - \tilde{\epsilon}_s)}{Z_s(n-1, E - \tilde{\epsilon}_s) + Z_s(n, E)} = \frac{1}{1 + \frac{Z_s(n, E)}{Z_s(n-1, E - \tilde{\epsilon}_s)}} \quad (19)$$

Here, two “partial” partition functions $Z_s(n, E)$ and $Z_s(n-1, E - \tilde{\epsilon}_s)$ are introduced. In the first one, the summation is taken over all single-particle states of n particles with the orbital s excluded, $Z_s(n, E) = \sum_k' F(E_k - E)$. Correspondingly, the sum in $Z_s(n-1, E - \tilde{\epsilon}_s)$ is taken over the states of $n-1$ particles with the orbital s excluded. The latter sum appears from the terms for which the orbital s is filled ($n_s = 1$), thus, we should add the energy $\tilde{\epsilon}_s \equiv E_k(n) - E_k(n-1)$ of this orbital to the energy $E_k(n-1)$ of the basis state $|k\rangle$ defined by $n-1$ particles. Since the F -function depends on the difference $E_k + \tilde{\epsilon}_s - E$ only, the adding term $\tilde{\epsilon}_s$ to $E_k(n-1)$ is the same as its subtraction from the total energy E . Note, that this term is defined by

$$\tilde{\epsilon}_s = \epsilon_s + \sum_{p \neq s} u_{sp} n_p^{(k)} \quad (20)$$

where ϵ_s is the energy of a single-particle state and u_{sp} is the diagonal matrix element of the two-body residual interaction. By taking $\tilde{\epsilon}_s$ independent of k we assume that the averaging over the basis states near the energy E is possible, in fact, this is equivalent to a local (at a given energy) mean field approximation.

One should stress that this approximation is the most important when applying the model (1) to realistic systems. For example, for Ce atom there are orbitals from different open sub-shells (e.g. $4f$ and $6s$) which are quite close in energies, however, they have very different radius. As a result, the Coulomb interaction between the corresponding electrons is very different [9]. In this case the interaction terms in Eq.(20) strongly depend on the occupation numbers of other particles, which means that there is no good mean field approximation. As a result, the equilibrium distribution for occupation numbers is very different from the Fermi-Dirac distribution [9]. However, the F -distribution (5) for occupation numbers is valid. In other cases like random two-body interaction model [5,3,8] or nuclear shell model [4], such a local mean field approximation is quite accurate.

For large number $n \gg 1$ of particles distributed over $m \gg 1$ orbitals, the dependence of Z_s on n and $\tilde{\epsilon}_s$ is very strong since the number of terms N in the partition function Z_s is exponentially large, $N = \frac{m!}{(m-n)!n!}$. Therefore, to make the dependence on arguments smooth, one should consider $\ln Z_s$ instead of Z_s . In this case one can obtain

$$\ln Z_s(n - \Delta n, E - \tilde{\epsilon}_s) \approx \ln Z_s(n, E) - \alpha_s \Delta n - \beta_s \tilde{\epsilon}_s$$

$$\alpha_s = \frac{\partial \ln Z_s}{\partial n}; \quad \beta_s = \frac{\partial \ln Z_s}{\partial E}; \quad \Delta n = 1 \quad (21)$$

This leads to the distribution of the Fermi-Dirac type,

$$n_s = \frac{1}{1 + \exp(\alpha_s + \beta_s \tilde{\epsilon}_s)} \quad (22)$$

If the number of substantially occupied orbitals in the definition of Z_s is large, the parameters α_s and β_s are not sensitive as to which particular orbital s is excluded from the sum and one can assume $\alpha_s = \alpha \equiv -\mu/T$, $\beta_s = \beta \equiv 1/T$ as in the standard Fermi-Dirac distribution. Then, the chemical potential μ and temperature T can be found from the conditions of fixed number of particles and fixed energy,

$$\sum_s n_s = n \quad \sum_{s>p} u_{sp} n_s n_p = \sum_s n_s (\epsilon_s + \tilde{\epsilon}_s)/2 = E \quad (23)$$

Note, that the sums in (23), (20) containing the residual interaction u_{sp} can be substantially reduced by a proper choice of the mean field basis (for instance, the terms u_{sp} can have different signs in such a basis). In practice, the values ϵ_s and $\tilde{\epsilon}_s$ may be very close. Since in the above expressions (23) the non-diagonal matrix elements of the interaction are not taken into account, one can expect that the distribution of occupation numbers defined by these equations gives a correct result if the interaction is weak enough (ideal gas approximation). However, we can show (see Section 8) that, in fact, even for strong interaction the Fermi-Dirac distribution can be also valid if the total energy E is corrected in a proper way, by taking into account the increase of the temperature due to statistical effects of interaction.

One should also note that somewhat similar procedure transforms the canonical distribution (7) into the Fermi-Dirac distribution (see e.g. [10]) in the case of many non-interacting particles (ideal gas). It is curious that the Fermi-Dirac distribution is very close to the canonical distribution (7) even for very small number of particles ($n = 2$), provided the number of essentially occupied orbitals is large (which happens for $T \gg \epsilon$ or $\mu \gg \epsilon$). In fact, this is a result of a large number of “principal” terms in the partition function Z_s which allows us to replace α_s by α in the term $Z_s(n, T)/Z_s(n-1, T) \equiv \exp(\alpha_s + \beta T)$ in the canonical distribution (7) (compare with (19)).

More accurate consideration shows, however, that the temperature T in the Fermi-Dirac distribution is different from that in the canonical distribution. Indeed, using the expansion $\alpha_s = \alpha(\epsilon_F) + \alpha'(\epsilon_s - \epsilon_F)$ one can obtain the relation between the Fermi-Dirac (β_{FD}) and canonical (β) inverse temperatures, $\beta_{FD} = \beta + \alpha' \epsilon_F$. Concerning the chemical potential, its definition also changes, $-\mu/T = \alpha(\epsilon_F) - \alpha' \epsilon_F$. This fact is confirmed by our numerical simulations for an isolated system with few interacting Fermi-particles [5,3,8]. Namely, for the same total energy E of the system, the canonical and Fermi-Dirac distributions give the same distribution n_s defined, however, by different temperatures since they are determined by different equations (8) and (23).

The closeness of these two distributions for any number of particles is not so surprising in the presence of the thermostat, where even one particle is in the equilibrium. To the contrary, for isolated systems with small number of particles the applicability of the Fermi-Dirac distribution is not obvious. To answer this question, one needs to analyze the role of interaction in the creation of an equilibrium distribution.

V. ANALYTICAL CALCULATION OF OCCUPATION NUMBERS IN FINITE SYSTEMS

The advantage of the approach developed in this paper is that if we know the shape of eigenstates in the many-particle basis of non-interacting particles (the F -function) and the unperturbed density of states $\rho_0(E)$, one can analytically calculate the distribution of the occupation numbers n_s .

In order to calculate the occupation numbers n_s , we use the expression (19) containing two partial partition functions $Z_s(n, E)$ and $Z_s(n-1, E-\epsilon_s)$ which correspond to systems with n and $n-1$ particles, with the orbital s is excluded from the set of single-particle states. The partition function can be found from the relation

$$Z = \sum_k F(E_k - E) \approx \int \rho_0(E_k) F(E_k - E) dE_k \quad (24)$$

The density of unperturbed states $\rho_0(E_k)$ in a system of n particles distributed over m single-particle states (orbitals) was shown to be close to the Gaussian (see for example, [6,7,11]):

$$\rho_0(E_k) = \frac{N}{\sqrt{2\pi\sigma_0^2}} \exp\left(-\frac{(E_k - E_c)^2}{2\sigma_0^2}\right) \quad (25)$$

with E_c as the center of the energy spectrum and N as the total number of states. Let us assume that the shape of eigenstates F - is given by the Gaussian, too:

$$F(E_k - E) = \frac{1}{\sqrt{2\pi(\Delta E)^2}} \exp\left(-\frac{(E_k - E)^2}{2(\Delta E)^2}\right) \quad (26)$$

Here the variance $(\Delta E)^2$ is defined by Eqs.(55,56), and $E = E^{(i)} + \Delta_1^{(i)} = H_{ii}$ (see Appendix 1).

As was found, Gaussian shape of eigenstates (apart from long tails) occurs in realistic systems like Ce atom [2] and heavy nuclei [12]. Recently, the form of the F -function in dependence on the perturbation has been studied in details [13] in the model of Wigner Band Random Matrices, as well as in the random two-body interaction model [8] (see also nuclear calculations [14,15]). In particular, it was discovered, that the gaussian-type shape happens when the interaction is large enough, namely, when the Breit-Wigner width $\Gamma = 2\pi\rho V^2$ is comparable with the root-mean-square width ΔE (an effective band width of a Hamiltonian matrix).

By performing the integration in Eq.(24) one gets

$$Z(E) = \frac{N}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(E - E_c)^2}{2\sigma^2}\right) \quad (27)$$

where $\sigma^2 = \sigma_0^2 + (\Delta E)^2$ (it coincides with the variance of the perturbed spectrum). In order to calculate the occupation numbers n_s , we use the expression (19). For this, one needs to find the partial partition functions $Z_s(n, E)$ and $Z_s(n-1, E - \epsilon_s)$ corresponding to n and $n-1$ particles with the orbital s is excluded from the set of single-particle states. Now we have to calculate the number of states N_s and the center E_{cs} for these truncated systems,

$$N_s(n, m-1) = \frac{(m-1)!}{(m-1-n)!n!}$$

$$N_s(n-1, m-1) = \frac{(m-1)!}{(m-n)!(n-1)!}$$

$$E_{cs}(n) = \overline{\epsilon_{-s}} n; \quad E_{cs}(n-1) = (\overline{\epsilon_{-s}})(n-1)$$

$$\overline{\epsilon_{-s}} = \frac{\sum_{p \neq s} \epsilon_p}{m-1}$$

The variance σ_{0s} of the energy distributions can be estimated as

$$\sigma_{0s}^2(n) \approx \sigma_{1s}^2 n; \quad \sigma_{0s}^2(n-1) \approx (\sigma_{1s}^2)(n-1)$$

where σ_{1s}^2 is the variance of single-particle spectrum with the excluded orbital s . Here, for simplicity, we have neglected the Pauli principle which is valid for $m \gg n$. More accurate calculation can be easily done with the use of calculator. As a result, the distribution of occupation numbers has the form

$$\begin{aligned} \overline{n_s}(E) &= \frac{1}{1+R} \\ R &= \frac{m-n}{n} \frac{\sigma_s(n-1)}{\sigma_s(n)} \\ &\times \exp \left[-\frac{(E - E_{cs}(n))^2}{2\sigma_s^2(n)} + \frac{(E - \epsilon_s - E_{cs}(n-1))^2}{2\sigma_s^2(n-1)} \right] \end{aligned} \quad (28)$$

where $\sigma_s^2 = \sigma_{s0}^2 + (\Delta E)^2$.

It is instructive to compare this result with the Fermi-Dirac distribution which is valid for large number of particles. In this case $R = \exp((\epsilon_s - \mu)/T_{th})$ where $T_{th} = \sigma^2/(E_c - E)$ is the thermodynamic temperature which is discussed below, see (33). The chemical potential μ in this case should be calculated numerically to fix the total number of particles n . The data are reported

in Fig.1. One can see that Eq.(28) predicts occupation numbers in perfect agreement with the numerical experiment.

Finally, note that the same method can be used to solve another problem: to find the distribution of the occupation numbers $n_s(T)$ in finite systems of interacting particles in the thermal bath with the temperature T . For such a case, it is enough to replace the F -function by the canonical average $F(T, E_k)$, see (12). In fact, it is the method for taking into account the “random” interaction in the canonical distribution. The result for the occupation numbers $n_s(T)$ can be obtained from (28) by replacing $\sigma_s^2 \rightarrow 2\sigma_s^2$ and $E \rightarrow E_m + \Delta_1(E_m)$ where $E_m = E_c - \sigma^2/T$ and Δ_1 is a small correction, see Appendix 1.

VI. PARTICLES AND QUASI-PARTICLES, ROLE OF SINGLE-PARTICLE SPREADING WIDTH

In previous sections we have discussed the distribution of occupation numbers for real particles distributed over given orbitals. At the same time, there exist traditional approach which is based on the notion of “quasi-particles”. It allows to incorporate the effects of interaction in terms of single-particle states and goes beyond the mean-field approximation. As is well known, the interaction leads to the spreading width γ_s for single-particle orbitals. It also results in the shift of average energies, $\tilde{\epsilon}_s = \epsilon_s + \delta\epsilon_s$. According to our numerical data ([5]) for the random two-body interaction model, the shifts $\delta\epsilon_s$ turn out to be, in average, smaller than γ_s and for this reason one can take into account the effect of spreading widths γ_s only.

Here we would like to analyze the role of the spreading widths for the distribution of occupation numbers and compare with our approach where the interaction is taken into account in terms of many-body states. For this, let us average the standard Fermi-Dirac occupation numbers n_s over the energy interval γ_s :

$$n_s = \int_{\epsilon_s - \gamma_s/2}^{\epsilon_s + \gamma_s/2} n(\epsilon) \frac{d\epsilon}{\gamma_s} = 1 - \frac{T}{\gamma_s} \ln \left[\frac{1 + \exp\left(\frac{\epsilon_s + \gamma_s/2 - \mu}{2T}\right)}{1 + \exp\left(\frac{\epsilon_s - \gamma_s/2 - \mu}{2T}\right)} \right] \quad (29)$$

where

$$n(\epsilon) = \frac{1}{1 + \exp\left(\frac{\epsilon - \mu}{T}\right)} \quad (30)$$

It seems, this is the simplest form of the Fermi-Dirac distribution for the “quasi-particles” with finite spreading widths. One can check that in the limit $\gamma_s = 0$ the Fermi-Dirac expression (30) with $n_s = n(\epsilon_s)$ is recovered.

To test the sensitivity of the occupation numbers to the values of the spreading widths γ_s , we have solved equations (23) for chemical potential and temperature (for a

given energy of our isolated system) using the standard expression (30), and compared the result with that obtained by using the expression (29), see details in [5]. The data have revealed that the chemical potential practically does not change, while there is a noticeable decrease of the temperature, $T(\gamma \neq 0) < T(\gamma = 0)$. The striking result is that the two curves for the occupation numbers (29) and (30) coincide with a high accuracy, namely, $n_s(\epsilon_s, \gamma, T) \approx n_s(\epsilon_s, \gamma = 0, T + \Delta T) \equiv n_s(\epsilon_s, \tilde{T})$. This means that the temperature mimics the effect of the spreading widths, the phenomenon which is far from being trivial. The shift of the temperature for $\gamma \ll \mu$ can be estimated analytically as $\Delta T \approx \gamma^2/16T$.

The above result indicates that one should not worry about the finite width of single-particle orbitals (“quasi-particles”) when calculating the occupation numbers.

VII. THERMODYNAMICS OF SMALL SYSTEMS

One of the important questions is about thermodynamical description of isolated systems of interacting particles. In any thermodynamical approach one needs to define, in a consistent way, such quantities as entropy, temperature and equation of state. Different definitions of the entropy and temperature have been recently discussed [16] (see also [17]) in application to shell models of heavy nuclei. In particular, it was found that for a realistic residual interaction, different definitions of temperatures lead to the same result. Below, we analyze few definitions of the temperature and entropy and show that for small number of interacting particles they may give quite different results.

Standard thermodynamical definitions of the entropy S_{th} and temperature are based on the density of states $\rho(E)$,

$$S_{th} = \ln \rho(E) + \text{const} \quad (31)$$

$$\frac{1}{T_{th}} = \frac{dS_{th}}{dE} = \frac{d \ln \rho}{dE} \quad (32)$$

In fact, such a definition of the temperature follows from the estimate of the position of maximum of the canonical averaging function $\Phi_T(E)$, see (10) and (13). It is usually assumed that the position of its maximum E_m coincides with the energy E of a system. One should stress that in the above definitions $\rho(E)$ is the perturbed density of states, therefore, the interaction is essentially taken into account.

However, for finite isolated systems with the fixed energy E , the definition of the temperature given by the relation $\langle E \rangle_T = E$ (see Eq.(8)) seems to be more natural. Here the averaging is performed over the canonical distribution (7). Since the width Δ_T of the canonical averaging function $\Phi_T(E)$ is not zero, the two definitions of the temperature, (32) and (8) give, in principal, different

results. Indeed, in the case of the Gaussian form of $\rho(E)$ the value of T_{th} given by (32) takes the form (see also [16]),

$$T_{th} = \frac{\sigma^2}{E_c - E} \quad (33)$$

where E_c and σ are the center and the width of the distribution $\rho(E)$.

On the other hand, direct evaluation of the relation (8) leads to the following definition of the temperature,

$$T_{can} = \frac{\sigma^2}{E_c - E + \Delta} \quad (34)$$

Here, the shift Δ is given by the expression

$$\Delta = \frac{\sigma}{K} \left[e^{-\frac{(E_{\min} - E_m)^2}{2\sigma^2}} - e^{-\frac{(E_{\max} - E_m)^2}{2\sigma^2}} \right] \quad (35)$$

where

$$K = \int_{x_{\min}}^{x_{\max}} \exp\left(-\frac{x^2}{2}\right) dx \approx \sqrt{2\pi};$$

$$x = \frac{E - E_m}{\sigma}; \quad E_m = E_c - \frac{\sigma^2}{T_{can}} \quad (36)$$

One can see that the shift Δ itself depends on the temperature and is proportional to the width $\Delta_T = \sigma$ of the function $\Phi_T(E)$. In the above relations, E_{\min} and E_{\max} are the low and upper borders of the energy spectrum. Note that the relation $\Delta = 0$ occurs at the center of the spectrum, therefore, the temperature in the upper part of the spectrum is negative (it is typical for systems with bounded spectrum, for example, for spin systems). In fact, our model (1) with finite number m of orbitals can be treated as the model of one open shell in atoms, nuclei, clusters, etc. However, in realistic many-body systems there are always higher shells which contribute to the density of states for higher energy. Thus, the density of states $\rho(E)$ is a monotonic function which results in the positive temperature. For such physical applications, the model (1) with finite number of orbitals is reasonable in the lower part of the energy spectrum where the influence of higher shells can be neglected.

One can also see that the difference between the two equations of state $T(E)$ defined by Eqs.(33) and (34), disappears for highly excited eigenstates (for which $E_m - E_{\min} \gg \sigma$), or in large systems with $n \gg 1$. Indeed, one can obtain, $E_c - E \sim n\sigma_1$, where σ_1 is the width of single-particle spectrum. On the other hand, according to the central limit theorem, the variance of total energy spectrum can be estimated as $\sigma_0^2 \approx \sum_n \sigma_1^2 = n\sigma_1^2$, therefore, the ratio $\sigma/(E_c - E) \sim 1/\sqrt{n}$ tends to zero at $n \rightarrow \infty$. Note, that in finite systems (atom, nucleus etc.) the number of valence particles (particles in an open shell) is not large. For example, for Ce atom we have $n = 4$ [2]

and in nuclear shell model [4] $n = 12$, therefore, the corrections to the thermodynamical temperature (32) can be significant, especially, for low energies. Here, we do not take into account particles from deep closed shells since their excitation energy is high and they do not contribute to the thermodynamical and statistical properties of systems (though they renormalize parameters of the Hamiltonian (1) describing the interaction between valence particles).

The energy dependence of temperatures T_{th} and T_{can} is shown in Fig.2. The data are given for the model of $n = 4$ interacting Fermi-particles distributed over $m = 11$ orbitals. The two-body interaction is taken to be completely random, given by the gaussian distribution of two-body matrix elements with $V = 0.12$; this value should be compared with the mean energy distance $d_0 = 1$ between the orbitals (single-particle energies), see details in [5,3,8]. The comparison of the thermodynamical temperature T_{th} defined by (33) with the “canonical” temperature (34) reveals quite strong difference in all the range of the rescaled energy $\chi = (E - E_{fermi})/(E_c - E_{fermi})$. To test our analytical expression for the canonical temperature T_{can} we have performed direct numerical calculation of the temperature according to (8) with the actual spectrum $E^{(i)}$ of the two-body random interaction (instead of the Gaussian approximation of $\rho(E)$). Numerical results well agree with the analytical expression (34).

The knowledge of the equation of state $E(T)$ gives the possibility to examine heat capacity of closed systems with finite number of interacting particles,

$$C = \frac{dE}{dT} = \frac{\sigma^2}{T^2} \left(1 + \frac{\partial \Delta}{\partial E_m} \right) \quad (37)$$

The second term in the above expression is a correction which vanishes for highly excited states or in large systems, however, it may be important in other situations.

Following the paper [16], we can also compare different definitions of entropy. Natural definition of the entropy in isolated systems can be directly related to the number of principal components N_{pc} in exact eigenfunctions.,

$$S_{EF} = \ln N_{pc} \quad (38)$$

In such a definition the entropy characterizes the complexity of a system (note, that for unperturbed “simple” states $N_{pc} = 1$ and $S_{EF} = 0$). There are several definitions of N_{pc} one of which is the so-called “entropy localization length” defined via the information entropy S_{inf} of eigenstates,

$$N_{pc} = \exp(S_{inf}) \quad (39)$$

where

$$\begin{aligned} S_{inf}(E) &= - \sum_k F_k(E) \ln F_k(E) \\ &\approx \int dE_k \rho(E_k) F(E_k - E) \ln F(E_k - E) \end{aligned} \quad (40)$$

Here we have used the F -function instead of $|C_k^{(i)}|^2$ in order to have smooth dependence of the entropy S_{inf} on the energy E . Another possibility is to find N_{pc} from the “inverse participation ratio”,

$$N_{pc}^{-1} = \sum_k (F_k(E))^2 \quad (41)$$

One more definition is $N_{pc}^{-1} = \max[F_k(E)] \approx F(E_k = E)$ which has been used in [2]. The difference between the above definitions of N_{pc} depends on a specific shape of $F_k(E)$, however, the values of N_{pc} differ from each other by some coefficient which is typically close to 1.

On the other hand, the estimate for N_{pc} can be obtained simply from the relation

$$N_{pc} \approx \frac{\Gamma}{D} = \Gamma \rho(E) \quad (42)$$

where Γ is the spreading width of the function $F_k(E)$ and D is the local mean spacing between many-particle energy levels. Thus, one can directly relate the number of principal components N_{pc} to the density of states $\rho(E)$,

$$S_{EF} = \ln N_{pc} \approx \ln \rho(E) + \ln \Gamma \quad (43)$$

One can see that the entropy S_{EF} found from exact eigenstates coincides with the thermodynamical entropy S_{th} if the second term in (43) does not depend on the energy. As is shown in Appendices 1-3, the spreading width Γ only weakly depends on the energy, in contrast to a very strong energy dependence of $\rho(E)$. The fact that the information entropy S_{inf} contains the term $\ln \rho$ was mentioned for the first time in [16]. One should stress that the above relations (42,43) are valid if N_{pc} is smaller than the size N of many-particle basis, $N_{pc} < N/2$. One has also to remind that systems under consideration are assumed to be in equilibrium, see discussion in Section 9.

VIII. INCREASE OF EFFECTIVE TEMPERATURE DUE TO STATISTICAL EFFECTS OF INTERACTION

In Section 4 we have shown that in the case of large number of particles, the distribution of occupation numbers is of the Fermi-Dirac form (22) if the local mean field approximation is valid. However, if one uses the expression (23) in order to find the chemical potential μ and temperature T , one can obtain inaccurate result. To demonstrate this, we have computed the distribution of occupation numbers n_s for the two-body random interaction model directly from exact eigenstates of the Hamiltonian matrix (1) defined in the basis of many-particle unperturbed states (see also [5,8]). These data for the “experimental” values of n_s are shown in Fig.3

by the histogram which is obtained by the average over a small energy window in order to smooth the fluctuations (also, an additional averaging over different realizations of the random two-body random interaction has been done). To compare with the standard Fermi-Dirac distribution, we have numerically solved Eqs.(23) in order to find the temperature and chemical potential. The resulting distribution of the occupation numbers n_s is shown in Fig.3 by circles. One should stress that the value of the energy E in (23) was taken the same as for the exact eigenstates from which actual distribution of n_s was computed, namely, $E \approx E^{(i)}$. The comparison of the actual distribution (histogram) with the theoretical one, see (23), reveals big difference for a chosen (quite strong) perturbation $V = 0.20$.

This discrepancy is due to the fact that the off-diagonal interaction is not taken into account in (23). In [5] it was pointed out that one can take into account statistical effects of interaction and to correct the total energy in (23) in the following way. Let us first consider the thermodynamical temperature T_{th} defined by (33). As was mentioned above, see (18), one can represent the width of perturbed density of states $\rho(E)$ in the form $\sigma^2 = \sigma_0^2 + \overline{(\Delta E)^2}$ where σ_0 relates to the unperturbed density and ΔE is an increase of the width of the energy spectrum due to the interaction. Thus, the temperature at a given energy E increases due to the interaction as follows

$$T = T_0 + \Delta T \approx \frac{\sigma_0^2}{E_c - E} + \frac{\overline{(\Delta E)^2}}{E_c - E} \quad (44)$$

resulting in the following relation,

$$\Delta T/T_0 = \overline{(\Delta E)^2}/\sigma_0^2 \quad (45)$$

The explanation of this increase of the temperature was given in [8] and reads as follows. Since the density of states rapidly increases with the energy E , the number of higher basis states admixed to an eigenstate by the interaction is larger than the number of lower basis states. An extreme example is the ground eigenstate, which contains basis components of higher energies only. As a result, the mean energy

$$\langle E_k \rangle_i = \sum_k E_k F_k^{(i)} \approx \int E_k F_k^{(i)} \rho_0(E_k) dE_k \quad (46)$$

of the components in an exact eigenstate $|i\rangle$ is higher than the eigenvalue $E^{(i)}$ corresponding to this eigenstate (we consider here eigenstates in the lower part of the spectrum only). There is another effect which gives the increase of $\langle E_k \rangle_i - E^{(i)}$ even if the density of states does not depend on the energy. Due to repulsion between the energy levels, the eigenvalues move down for this part of the spectrum, therefore, the difference between $\langle E_k \rangle_i$ and $E^{(i)}$ increases due to the interaction. This second effect shifts the “center” of the function $F_k^{(i)} = F(E_k - E^{(i)})$

. One should stress that all effects leading to the above shift of the energy are automatically taken into account in the relation (46). Thus, one can analytically calculate this shift $\Delta E = \langle E_k \rangle_i - E^{(i)}$ from the equation (46). For this, one needs to know the unperturbed density of states and the form of the F -function. The evaluation of the shift ΔE has been done in [8] by assuming some form for the F -function which is valid in a wide range of the interaction strength V ,

$$\begin{aligned} \Delta E = \langle E_k \rangle_i - E^{(i)} &= \frac{d \ln \rho_0}{dE} \overline{(\Delta E)^2} = \frac{1}{T_0} \overline{(\Delta E)^2} \\ &= \frac{\overline{(\Delta E)^2}}{\sigma_0^2} (E_c - E) \end{aligned} \quad (47)$$

Now, in order to obtain the corresponding increase of the temperature, one should insert the shifted energy $E \equiv \langle E_k \rangle_i = E^{(i)} + \Delta E$ into the equation for the temperature,

$$\begin{aligned} T = T_0 + \Delta T &= \frac{\sigma_0^2}{E_c - E^{(i)} - \Delta E} \\ &\approx \frac{\sigma_0^2}{E_c - E^{(i)}} + \frac{\overline{(\Delta E)^2}}{E_c - E^{(i)}} \end{aligned} \quad (48)$$

One can see that Eq.(48) is consistent with Eq.(44) for $\overline{(\Delta E)^2} \ll \sigma_0^2$.

Thus, to find correct values for the occupation numbers in the Fermi-Dirac distribution, we should substitute the increased energy $E = E^{(i)} + \Delta E = \langle E_k \rangle_i$ into equations (23) for the chemical potential and temperature. The resulting shift of the temperature and chemical potential leads to the distribution of the occupation numbers shown in Fig.3 by diamonds. As one can see, such a correction gives a quite good correspondence to the numerical data.

To check the analytical prediction (47) for the shift ΔE , we have calculated this shift directly by comparing the energy $E^{(i)}$ of exact eigenstates with the energy $\langle E_k \rangle_i$. The latter has been computed from the exact relation $\langle E_k \rangle_i = \sum_k E_k \left| C_k^{(i)} \right|^2$ (compare with (46)). The comparison of these data (circles in Fig.4) with Eq. (47) (straight full line) shows a good agreement, if to neglect strong fluctuations around the global dependence. These fluctuations are due to fluctuations in the components of specific exact eigenstates $|i\rangle$ (note, that the presented data correspond to the individual eigenstates, without any additional averaging).

Finally, we would like to note that the described above method can be also used to solve the “canonical” problem of finding the distribution of the occupation numbers for a system of interacting particles in the thermal bath. Indeed, the distribution $n_s(T)$ for the “ideal” gas is given by the canonical distribution, or more simple, by the Fermi-Dirac distribution if the number of particles $n \gg 1$ (in practice, $n > 2$ is enough). The increase

of “kinetic” energy due to the random residual interaction is given by $\Delta_E = \overline{(\Delta E)^2}/T$, see Eq.(47). Then, one can find the effective temperature which corresponds to the same increase of the average “kinetic” energy in the ideal gas. It can be done by the differentiation of $T^{-1} = dS/dE$, where S is the entropy, $S = \ln \rho_0 + \text{const}$. The result reads as

$$\Delta T = -T \frac{d^2 \ln \rho_0}{dE^2} \overline{(\Delta E)^2} \quad (49)$$

For the Gaussian shape of the level density $\rho_0(E)$ it coincides with (45). Thus, we can use the Fermi-Dirac distribution with the effective temperature $T_{eff} = T + \Delta T$ in order to describe “randomly” interacting particles (for $\Delta T \ll T$) in the heat bath.

IX. CRITERIA FOR THE ONSET OF CHAOS, EQUILIBRIUM AND THERMALIZATION

The theory presented above is based on the notion of chaos in terms of statistical properties of compound eigenstates. Typically, the onset of quantum chaos is associated with large number of components in the eigenstates. However, as we can see below, this condition is not enough for the emergence of equilibrium distributions and, in essence, there are different regimes of “chaos”. Here, we analyze the conditions under which the possibility of statistical description of isolated systems of interacting particles can be directly related to statistical properties of eigenstate components.

Let us start with the condition of a large number of principal components N_{pc} provided there is an equilibrium distribution of the components of eigenstates. For the relatively small interaction, the distribution of the components has the Breit-Wigner form,

$$F_k^{(i)} \equiv \overline{|C_k^{(i)}|^2} = \frac{1}{N_{pc}} \frac{\Gamma_{BW}^2/4}{(E_k - E^{(i)})^2 + \Gamma_{BW}^2/4} \quad (50)$$

Here, the value $N_{pc} = \frac{\pi \Gamma_{BW}}{2D}$ is defined by the normalization condition and $D = \rho^{-1}(E)$ is the mean spacing between energy levels, and spreading width is given by

$$\Gamma_{BW} = 2\pi \frac{V^2}{d_f} \quad (51)$$

where V^2 is the mean squared value of matrix elements of the two-body interaction, see (1). In the denominator d_f stands for the mean energy spacing of those basis components to which a particular basis state $|k\rangle$ can “decay” due to direct two-body interaction, see details in Appendix 3. Thus, the condition $N_{pc} \gg 1$ reads

$$N_{pc} = \frac{\pi^2 V^2}{d_f D} \gg 1$$

or

$$V \gg \frac{1}{\pi^2} \sqrt{d_f D} \quad (52)$$

However, as was pointed out in [18] (see also [19,20,21]), there is a phenomenon of “localization in the Fock space” which means that the states with different number of excited particles do not mix with each other. This situation occurs when $V < d_f$ (with some logarithmic corrections). This means that in order to have an ergodic distribution for the eigenstate coefficients resulting in the equilibrium distribution of occupation numbers for individual eigenstates, one needs both the conditions, $V > d_f$ and (52). Since d_f is typically much bigger than D , the condition $V > d_f$ is stronger than (52).

Let us now discuss the properties of eigenstates and distribution of occupation numbers in dependence on two above parameters, V/d_f and N_{pc} . Since the value of N_{pc} increases with an increase of V , we first start with a very weak interaction for which exact eigenstates have only a few relatively large components ($N_{pc} \sim 1$). In such a case the eigenstates are strongly localized in the unperturbed basis and, therefore, can be described by conventional perturbation theory. This situation is quite typical for lowest eigenstates (where the density of states is small) even if for higher energies the eigenstates can be considered as very “chaotic” ($N_{pc} \gg 1$). We term this region (I) as a region of strong (perturbative) localization.

The second region (II) is characterized by an “initial chaotization” of exact eigenstates and corresponds to a relatively large, $N_{pc} \gg 1$ number of principal components and $V < d_f$. The latter condition is essential since it results in very strong (non-Gaussian) fluctuations of components $C_k^{(i)}$ [22] for the fixed energy $E^{(i)}$ of compound state $|i\rangle$. Such a type of fluctuations reflects itself in a specific character of eigenstates, namely, they turn out to be “sparsed”. As a result, the number of principal components can not be estimated as $N_{pc} \approx \Gamma/D$, as is typically assumed in the literature. Let us note that the energy width Γ of eigenstates is still close to the expression (51).

The above specific properties of compound states can be explained by the perturbation theory in the parameter V/d_f . Indeed, in the zero order approximation an eigenstate $|i\rangle$ coincides with a basis state $|k_0\rangle$ for which the particles occupy definite orbitals. In the first order in V/d_f the eigenstate $|i\rangle$ is constructed by those basis states $|k_1\rangle$ which can be obtained from $|k_0\rangle$ by moving one or two particles (due to the two-body character of the interaction). As a result, the coefficients of the state $|i\rangle$ can be estimated as $C_{k_1}^{(i)} = V_{k_0, k_1} / (E^{(i)} - E_{k_1})$. If the matrix elements V_{k_0, k_1} are Gaussian variables, for the fixed spacing $|E^{(i)} - E_{k_1}|$ the coefficients $C_k^{(i)}$ are also distributed according to the Gaussian.

The situation is completely different in higher orders. For example, in the second order we have $C \equiv C_{k_2}^{(i)} = \sum_{k_1} V_{k_0, k_1} V_{k_1, k_2} / ((E^{(i)} - E_{k_1})(E^{(i)} - E_{k_2}))$ and the distribution $P(C)$ (for the fixed $|E^{(i)} - E_{k_2}|$) is close to

the Lorentzian, namely, $P(C) \sim C_{cr}/C^2$ for $C_{cr} < C < 1$ where $C_{cr} \sim V^2/d_f^2$ [23,22]. Long tails in the distribution $P(C)$ are due to the possibility of small values of the denominator $E^{(i)} - E_{k_i}$ in intermediate states. The higher orders r of the perturbation theory give stronger fluctuations (with additional logarithm in $P(C)$) because of large number of small denominators. Another type of even stronger fluctuations result from very different nature of many-body basis states with close energies. Namely, the states with nearly the same energy can differ by a large number of moved particles in order to obtain the corresponding states. Therefore, the transition into close (in energies) states appear in different orders of the perturbation. Therefore, the fluctuations of the components C appear to be abnormal, without obeying the standard central limit theorem. In particular, the above effect leads to very large fluctuations in the distribution of the occupation numbers n_s , as a function of the energy E of compound states. Specifically, the fluctuations do not decrease as $N_{pc}^{-1/2}$, for example, if $P(C) \sim 1/C^2$ the fluctuations of $n_s(E)$ do not depend on N_{pc} at all for $N_{pc} < 1/C_{cr}$ (see, for example, [23]).

As an example, one can take the two-body random interaction model (1) with $n = 4$ particles and $m = 11$ orbitals and very weak perturbation $V/d_0 \approx 0.02$ where d_0 is the mean level spacing between single-particle energy levels, see Fig.5. One can see that the “experimental” distribution of occupation numbers has nothing to do with the Fermi-Dirac distribution (full diamonds), it turns out to be even the non-monotonic function of the energy ϵ_s of orbitals (see also [5]). Note that the averaging procedure used in Fig.5 has not wash out the fluctuations in n_s .

With further increase of the interaction, where $N_{pc} \gg 1$ and $V > d_f$, the region (III) of the equilibrium for the F -distribution (5) emerges. In this region the fluctuations of the eigenstate components $C_k^{(i)}$ are of the Gaussian form [22] which leads to small fluctuations of the occupations numbers n_s in accordance with the central limit theorem for the sum (3), $\Delta n_s/n_s \sim N_{pc}^{-1/2} \ll 1$ for $n_s \sim 1$. One should stress that in this region the value of N_{pc} is given by the common estimate, $N_{pc} \sim \Gamma/D$. As a result, the distribution of occupation numbers changes slightly when changing the energy of a system. Such a situation can be naturally associated with the onset of thermal equilibrium, though the form of the distribution n_s can be quite different from the Fermi-Dirac distribution. In this case, the F -distribution (5) gives a correct description of an actual distribution of occupation numbers in isolated quantum systems of interacting particles. One can see that the equilibrium distribution for the occupation numbers arises for much weaker condition compared to that needed for the Fermi-Dirac distribution. Since the energy interval d_f between two-particle-one-hole energy levels is small, it is enough to have a relatively weak residual interaction $V > d_f$ in order to have the equilibrium distribution (note, that the value of d_f decreases

rapidly with the excitation energy, see Appendix 3).

Next region (IV) is where the canonical distribution (7) occurs; for this case in addition to the equilibrium, one needs to have large number of particles, $n \gg 1$. If, also, the condition $\Gamma \ll nd_0$ is fulfilled, the standard Fermi-Dirac distribution is valid with a proper shift of the total energy due to the interaction, see Section 8. Typically, this region is associated with the onset of the canonical thermalization (see, for example, [16]).

In practice, the condition (IV) of the canonical thermalization is not easy to satisfy in realistic systems like atoms or nuclei since n in the above estimates is, in fact, the number of “active” particles (number of particles in a valence shell) rather than the total number of particles. Thus, the description based on the F -distribution (5) which does not require the canonical thermalization condition (IV), is more accurate.

The above statements are confirmed by the direct numerical study of the two-body random interaction model [5,8] with few particles when changing the interaction strength V/d_0 . If, instead, we increase the number of particles keeping the interaction small, $V \ll d_0$, the distribution (5) tends to the Fermi-Dirac one as it is expected for the ideal gas, see [8].

Finally, we discuss the transition to mesoscopic systems. One can show that the result strongly depends on the dimensionality d of a system. Let us consider the case when the number of particles n is fixed, however, the size l of a system increases. Then, the interval between single particle energy levels decreases as $d_0 \sim l^{-2}$. Since relative interaction between two particles decreases like $V \sim l^{-d}$, one can get, $V/d_0 \sim l^{-(d-2)}$. Thus, for $d = 1$ one has $V \gg d_0$ which means that strong mixing (chaos) starts just from the ground state. This is in accordance with the absence of a gap in the distribution of occupation numbers in 1D case (the so-called Luttinger liquid). To the contrary, in the 3D case we have $V \ll d_0$; this means that an admixture of the higher states to the ground state can be considered perturbatively, which is consistent with the non-zero gap at $T = 0$. One can see that the transition between regular region (I) and the equilibrium (region III) in the 3D case occurs for high states when $V \geq d_f$. Recently, the question of this transition has been studied in [18,20,21].

X. CONCLUSION

In this paper we have developed statistical approach to isolated finite systems of interacting particles, which plays the same role as the canonical approach for systems in equilibrium with the thermal bath. It can be applied to complex many-body systems like compound nuclei, rare-earth actinide atoms, atomic clusters, quantum dots, etc. The key point of this approach is a new kind of the partition function which is defined to the shape of compound states (F -function) in the many-

particle basis of a system without residual interaction (Slater determinants). It allows to calculate mean values of different operators as a function of the total energy E of a system. As an example, we have calculated the occupation numbers $n_s(E)$, which may be compared with the standard canonical approach giving $n_s(T)$ where T is the temperature of an open system. In large systems (thermodynamical limit) the distribution of occupation numbers n_s tends to the canonical distribution with the temperature $T^{-1} = d(\ln \rho) / dE$ where $\rho(E)$ is the energy level density.

Another important area of applications of our approach is the calculation of non-diagonal matrix elements (transition amplitudes) between the eigenstates of complex many-body systems. We would like to point out that the approach can be also used for solving traditional problem of calculations of mean values of operators in open systems of interacting particles in the thermostat.

The suggested approach is entirely based on the statistical properties of chaotic compound states which are due to the two-body interaction between the particles. For relatively strong interaction the number of components of compound states is typically large and these components can be treated as random variables, provided the two-body interaction matrix elements are “complex” enough.

The essential question is under which conditions the above approach is valid in systems with the two-body random interaction. Note, the randomness of the matrix elements itself is not enough for the onset of the equilibrium in the system since statistical properties of compound eigenstates essentially depend on such parameters as the relative strength of the interaction, excitation energy, number of particles and orbitals (single-particle states participating in the energy exchange), etc. In particular, even if the number of principal components in compound states is large, for not strong enough interaction the statistics of the components can be abnormal, leading to huge (non-Gaussian) fluctuations in the structure of the eigenstates. In such a case, there is no equilibrium in the system and standard statistical description is not valid. In this regime, our numerical data show that the distribution of the occupation numbers strongly fluctuates when slightly changing the total energy of the system. Therefore, the transition to the statistical equilibrium is far from being trivial in the systems with finite number of interacting particles. However, for larger interaction the fluctuations of the eigenstate component becomes normal (Gaussian) and the equilibrium occurs. In this situation the fluctuations of the occupation numbers $n_s(E)$ are relatively small and the F -function gives a correct result for the isolated finite systems even for small number of interacting particles (provided the number of principal components in the eigenstates is large).

The advantage of our approach, in comparison with direct calculations of complex quantum systems, is that we do not need to diagonalize huge Hamiltonian matrices in order to perform calculations of observables for

excited states. Indeed, for the full statistical description of such systems, one needs to know the average shape of the compound states (rather than the eigenstates themselves) and the unperturbed energy spectrum. Therefore, the problem of analytical description of the shape of eigenstates is the central point in the technical implementation of the approach. One should note that the average shape of eigenstates is the same as that of the local spectral density of states (LDOS), if the interaction is not extremely strong.

For small interaction the shape of the chaotic eigenstates is known to be well described by the Breit-Wigner form. However, in practice, this region is small if the number of particles is not very large. With an increase of the interaction strength, the average shape of the eigenstates (F -function) changes from the Breit-Wigner one to that close to the Gaussian with the exponential tails. As we have found (Appendix 1), the correct description of the shape requires two essential parameters. The first one is, in fact, the half-width of the F -function which is close to the Breit-Wigner half-width and for weak interaction is given by the Fermi Golden Rule. Another parameter is defined by the root-mean-square width of the F -function, or, the same, by an effective band-width of the Hamiltonian matrix in the energy representation.

In this paper we suggest the phenomenological expression for the F -function which is valid in a large region of the interaction strength and other parameters. This expression allows for the analytical and numerical calculations of different mean values and transition amplitudes. As one example, we have derived analytical expression for the distribution of the occupation numbers $n_s(E)$ in isolated systems of n interacting Fermi-particles distributed over m orbitals (we have used the simple Gaussian approximation of the F -function, see Section 5).

By making use of the F -function, we have also studied the validity of the standard Fermi-Dirac distribution for the description of finite systems of interacting Fermi-particles. As was found, the Fermi-Dirac distribution can provide reasonable approximation for both isolated and open (in the thermal bath) systems. However, the parameters of the Fermi-Dirac distribution have to be re-defined by taking into account the increase of the effective temperature which is due to the effects of the interaction. We calculated this increase of the temperature analytically and compared with the numerical experiments for the two-body random interaction model; the data show very good agreement.

One should stress that our approach gives more accurate result for n_s and has much wider region of the applicability, compared to the Fermi-Dirac distribution. Specifically, it is valid even in the region where the Fermi-Dirac distribution fails, for example, due to the small number of particles.

To conclude with, we would like to point out that similar approach may be also used for classical chaotic systems. Indeed, let us consider the system described by the Hamiltonian $H = H_0 + V$ where H_0 is the unper-

turbed (“simple”) Hamiltonian and V stands for “complex” interaction between particles. Assume that we know the distribution for some variable in the system described by H_0 , for example, the statistical average for the energy distribution of a single particle $n(\epsilon, E_0)$ where ϵ is the energy of the particle and E_0 is the total energy of the system. Then, one can calculate the effect of the interaction V by averaging of $n(\epsilon, E_0)$ over the unperturbed energy E_0 using the F -function, $n(\epsilon, E) = \int n(\epsilon, E_0) F(E, E_0) dE_0$. Here $F(E, E_0)$ gives the probability of different values of E_0 for a given value of E . As was indicated in [26] and checked numerically in [27,28], this classical F -distribution coincides with the shape of quantum eigenstates in the semiclassical region which turns out to be very wide. Thus, the knowledge of the shape of quantum eigenstates can be used for the classical calculations and vice versa.

Acknowledgements

The authors are thankful to Y.Fyodorov, G.Gribakin, M.Kuchiev, J.-L.Pichard, I.Ponomarev, V.Sokolov and O.Sushkov for the discussions; F.M.I. is very grateful to the staff of School of Physics, University of New South Wales for the hospitality during his visit when this work was done. This work was supported by the Australian Research Council. F.M.I. acknowledges the partial support by Grant No.94-2058 from INTAS.

Appendix 1. Structure of chaotic eigenstates and spreading function

For practical implementation of the above approach one needs to know the average shape of compound eigenstates (the F -function). One should stress that there is no simple analytical expression valid in a large range on the interaction strength V . For example, the popular Breit-Wigner expression (Lorentzian) is not good for obvious reason: it has infinite second moment. The question of an appropriate description of chaotic eigenstates in realistic many-body systems has been studied in detail for Ce atom [2]. In particular, it was found that good correspondence to the numerical data is given by two phenomenological expressions. The first one is $F(x) \sim \exp(-\sqrt{1+4x^2})$ where $x = (E_k - E)/\Gamma$ with E_k as the energy of a basis state $|k\rangle$ and Γ as the effective width of the distribution. This expression is close to the Gaussian at the central part and is exponential in the tails (see similar conclusions in [16] where nuclear shell model was studied).

Another expression which is more convenient for the analytical study is the so-called “squared” Lorentzian [2],

$$F(E_k - E) \sim \frac{1}{[(E_k - E)^2 + \frac{\Gamma^2}{4}]^2}; \quad E = E^{(i)} + \Delta_1^{(i)} \quad (53)$$

Here $\Delta_1^{(i)} \ll \Gamma$ is some small shift (see below) which in the zero approximation can be neglected, and E_k is defined by

$$E_k = H_{kk} = \sum_s n_s^{(k)} \epsilon_s + \sum_{s>p} u_{sp} n_s^{(k)} n_p^{(k)} \quad (54)$$

Since the “resonant” dependence $E_k - E^{(i)}$ of the spreading function $F_k^{(i)}$ for not extremely strong interaction is symmetric in indexes i and k , the value of $\Gamma = 2\sqrt{(\Delta E)^2}$ can be expressed in terms of the second moment of F using the following exact relation for the basis components, see Appendix 2,

$$(\Delta E)^2 \equiv \sum_i \left| C_k^{(i)} \right|^2 (E_k - E^{(i)})^2 = \sum_{p \neq k} H_{kp}^2 \quad (55)$$

with H_{kp} standing for non-diagonal Hamiltonian matrix elements defined by the residual interaction V . This allows us to find the second moment of the spreading function $F(E)$. For example, in the case of n particles distributed over m orbitals we have [3]

$$\left(\frac{\Gamma}{2} \right)^2 = \overline{(\Delta E)^2} = \frac{V^2}{4} n(n-1)(m-n)(3+m-n) \quad (56)$$

Here $V^2 = \overline{|V_{st \rightarrow pq}|^2}$ is the mean squared value of non-diagonal matrix elements of the two-body residual interaction.

Our detailed study of the two-body random interaction model [3,5,8] has revealed that the shape of the eigenfunctions. (as well as the local spectral density of states) strongly depends on the relative strength of the interaction. Namely, with an increase of the interaction V , the shape of the F -function changes its form from the Breit-Wigner one to the nearly Gaussian (see also [13]). It was found that for small residual interaction the shape of eigenstates has more complicated form, compared to (53), and should be characterized by two different widths. Indeed, the half-width of the F -distribution is given by the Fermi golden rule $\Gamma_{BW} = 2\pi v^2/d_f$ where v is the matrix element of the residual interaction coupling a particular basis component with other basis states $|f\rangle$ directly coupled by the two-body interaction, and d_f is the energy spacing between these basis states (see details in Appendix 3). On the other hand, there is the relation (56) which defines another width $\Gamma = 2\sqrt{(\Delta E)^2}$ via the second moment. One should stress that these two widths are parametrically different in the interaction, $\Gamma_{BW} \sim V^2$, and $\Gamma \sim V$. There is also the “non-resonant” energy dependence $F \propto \rho^{-1}$ (slow variation of the F -function due to the change of the density of states $\rho(E)$) which should be taken into account. This dependence follows from the estimate $F_{max} \sim N_{pc}^{-1} \sim \Gamma \rho$.

The above arguments allow us to find more universal expression for the spreading function F when $\Gamma_{BW} < \Gamma$ [8],

$$F_k^{(i)} \sim \frac{(\rho_0(E_k)\rho(E^{(i)}))^{-1/2}}{\left[(E_k - E)^2 + \frac{\Gamma^2}{4} \right] \left[(E_k - E)^2 + \frac{\Gamma_{BW}^2}{4} \right]} \quad (57)$$

Here we take into account the shift of the maximum of the F -function by the relation $E = E^{(i)} + \Delta_1^{(i)}$. The two parameters, Γ_1 and Γ_2 are directly related to the above two widths, $\Gamma_1 = \Gamma_{BW}$ and $\Gamma_2 = \Gamma^2/\Gamma_1$. The value of Γ_2 is found from the relation $\sum_i F_k^{(i)} (E^{(i)} - E_k)^2 = \overline{(\Delta E)^2} = \Gamma^2/4$ (see (56) and Appendix 2) by integration of (57) in the approximation $\rho = \text{const}$. Here and below we assume that the F -function is normalized, $Z = 1$. In the expression (56), $\rho_0(E_k)$ is the density of basis (unperturbed) states and $\rho(E^{(i)})$ is the density of compound states. We assume they are smooth functions of the energy and this energy dependence is slow in comparison with the “resonant” energy dependence on the scale Γ . Symmetric dependence on ρ_0 and ρ has been chosen in order to keep symmetry in indexes k and i in the F -function.

For very small V we have $\Gamma_1 \ll \Gamma_2$ (also, $\Delta_1^{(i)} \ll \Gamma_1$, see below), therefore, in the central part the F -distribution (57) has the Breit-Wigner shape with the width Γ_{BW} . Concerning the meaning of Γ_2 , it is the effective energy band width of the Hamiltonian matrix H , which is due to the two-body nature of the interaction. Indeed, the expression for Γ_2 is given by the estimate

$$\Gamma_2 = \frac{\Gamma^2}{\Gamma_{BW}} \approx \frac{d_f}{2\pi} n(n-1)(m-n)(m-n+3) \approx d_0(m-n) \quad (58)$$

which is independent of the interaction strength V . Here we have used expression (56) and the estimate of the average value $d_f \equiv d_0/M_f$ for high excited states (M_f here is the normalized density of those basis states which are directly connected to the chosen state, see details in Appendix 3). On the other hand, the typical band width $\Delta_H \equiv 2bd_0$ of the two-body interaction Hamiltonian matrix is about four times, $\Delta_H \approx 4(m-n)d_0$, of the energy needed to transfer the particle from the Fermi-level $\epsilon_F = nd_0$ to the highest available orbital $\epsilon_m = md_0$. Therefore, the estimate for Γ_2 reads as $\Gamma_2 \approx \Delta_H/4$.

Now, we can easily explain the form of the F -function (57) using the perturbation theory in the interaction V . First, let us consider the energy interval $\Gamma_{BW} < |E_k - E^{(i)}| < \Delta_H$. Within this interval, the basis state $|k\rangle$ can be coupled to the principal components of the state $|i\rangle$ in the first order of V , $|C_k^{(i)}|^2 \sim \left(\frac{V_{ik}}{E_k - E^{(i)}}\right)^2$. This quadratic decay agrees with the Breit-Wigner shape of the F -function. Outside the energy band Δ_H , for $\Delta_H < |E_k - E^{(i)}| < 2\Delta_H$, the basis state $|k\rangle$ can be coupled to the principal components of the state $|i\rangle$ in the second order of V , resulting in the dependence $|C_k^{(i)}|^2 \sim \left(\frac{V_{ik}}{E_k - E^{(i)}}\right)^4$. This corresponds to the tails of the squared Lorentzian shape (57). Therefore, our expression (57) seems to be good in a large energy interval and the second moment is finite which is important for applications. And finally, longer tails are described by

higher orders $\nu = \frac{|E_k - E^{(i)}|}{\Delta_H}$ of the perturbation theory,

$$\begin{aligned} |C_k^{(i)}|^2 &\sim \left(\frac{V_{ik}}{E_k - E^{(i)}}\right)^{2\nu} \\ &= \exp\left(-\frac{2|E_k - E^{(i)}|}{\Delta_H} \ln\left(\frac{|E_k - E^{(i)}|}{V}\right)\right) \end{aligned} \quad (59)$$

This explains the exponential tails of the F -function, see details in [2].

Numerical calculations [2,4,16,13] demonstrate that for stronger interaction V , the width of the spreading function F rapidly becomes linear in V (instead of the quadratic dependence in Γ_{BW}) and it is better to use (53). One can write the extrapolation expression both for small and large values of V (see also [16]):

$$\Gamma_1 = \frac{\Gamma_{BW}\Gamma}{\Gamma_{BW} + \Gamma} \quad (60)$$

As a result, for small V we have $\Gamma_{BW} \ll \Gamma$ and $\Gamma_1 = \Gamma_{BW} \sim V^2$ and for larger values $\Gamma_1 \approx \Gamma_2 \approx \Gamma \sim V \gg \Delta_1^{(i)}$. The critical value for this transition is given by the relation $\Gamma_{BW} = \Gamma = \Gamma_2 \sim \Delta_H$ and reads as $V_{cr} \approx d_f n(m-n)/(2\pi)$, see also (56). The estimate of the average value of $d_f \equiv d_0/M_f$ (see Appendix 3) far from the ground state gives $V_{cr} \sim d_0/n$. As was discussed in Section 9, the equilibrium distribution occurs for $V > d_f$, this results in a quite unexpected conclusion. Namely, the validity of the standard Breit-Wigner shape turns out to be very strongly limited since the region $1 < V/d_f \ll V_{cr}/d_f \approx n(m-n)/(2\pi)$ is practically absent for small number of particles n and orbitals m .

The shift $\Delta_1^{(i)}$ in (57) stands due to the level repulsion which forces eigenvalues $E^{(i)}$ in the lower half of the spectrum to move down. The mean field energies $E_k = H_{kk}$ do not include the non-diagonal interaction which leads to the repulsion, therefore, the “center” of the F -function is shifted by the value $\Delta_1^{(i)} = H_{ii} - E^{(i)}$ where H_{ii} is the diagonal matrix element of the Hamiltonian matrix. This shift $\Delta_1^{(i)}$ can be estimated from general arguments. Indeed, the shape of the density of states is the same for both interacting and non-interacting particles [6,7], with the same position E_c of the centers of $\rho_0(E)$ and $\rho(E)$ (due to the conservation of the trace of the Hamiltonian H). However, the variances of ρ_0 and ρ are different. This means that one can use the scaling relation ($D \rightarrow KD$) for the energy intervals D and find the scaling coefficient K from the relation between the variances, $\sigma^2 = \sigma_0^2 + (\Delta E)^2 = K^2 \sigma_0^2$ where $(\Delta E)^2$ is defined by (56). Since the center E_c for the energy level density $\rho(E)$ does not shift, one can obtain the following shift of the levels:

$$\Delta_1^{(i)} = (E_c - E^{(i)}) \left(\sqrt{1 + \frac{(\Delta E)^2}{\sigma_0^2}} - 1 \right) \quad (61)$$

The value of $\overline{(\Delta E)^2}$ is typically much less than σ_0^2 , therefore, one can get

$$\Delta_1^{(i)} \simeq \left(E_c - E^{(i)} \right) \frac{\overline{(\Delta E)^2}}{2(\sigma_0)^2} \quad (62)$$

Another way to obtain the shift $\Delta_1^{(i)}$ is related to the exact relation for the first moment of F , see Appendix 2,

$$E_k = \sum_i E^{(i)} F_k^{(i)} \approx \int F_k^{(i)} \rho(E^{(i)}) E^{(i)} dE^{(i)} \quad (63)$$

The substitution of the expression (57) into (63) results in the following value of the shift [8],

$$\Delta_1^{(i)} \simeq \frac{1}{2} \frac{d(\ln \rho)}{dE} \overline{(\Delta E)^2} \quad (64)$$

According to [6,7] (see also [11]) the shape of density of states for $m \gg n \gg 1$ is close to the Gaussian both for non-interacting and interacting particles with E_c and σ_0^2 as the center and the variance of the energy distribution $\rho_0(E)$ (respectively, σ^2 for $\rho(E)$). In this case the relation (64) gives the same estimate (62) for the shift $\Delta_1^{(i)}$.

The fact that the two different derivations of the shift $\Delta_1^{(i)}$ lead to the same result is far from being trivial since the assumptions for the two derivations of $\Delta_1^{(i)}$ are different. Indeed, the second derivation of (62) is based on the specific dependence of the eigenstate shape on the densities ρ_0 and ρ , unlike the general derivation of (61). One should stress that the specific form of the “resonant” energy dependence of the F -function (the denominator in (57) defined by the squared Lorentzian, Gaussian, etc.) is not important for Eq. (64) provided $\overline{(\Delta E)^2}$ is fixed. The only assumption in the above derivation is the possibility to expand the density $\rho(E)$ near the maximum of the F -function. In fact, above we have demonstrated that the non-resonant “distortion” factor $\xi \equiv (\rho_0(E_k) \rho(E^{(i)}))^{-1/2}$ in (57) is necessary.

Thus, the phenomenological expression for the shape of the F -function (57) is self-consistent. Note, that one can use other expressions for the F -function (see, for example, [13]), however, it should contain both the resonance term depending on $E_k - E^{(i)}$ and the density distortion factor ξ .

Appendix 2. Moments of the F -function and energy spectrum

Here we calculate the first and the second moment of the function $F_k^{(i)}$ over the perturbed spectrum $E^{(i)}$. Note, that the dependence of $F_k^{(i)}$ on the energy $E^{(i)}$ is known as the local spectral density of states (LDOS), or the “strength function”. On definition,

$$\begin{aligned} \langle E^{(i)} \rangle_k &= \sum_i E^{(i)} F_k^{(i)} \approx \sum_i \langle k, i |^2 E^{(i)} \\ &= \sum_{i,j} \langle k | i \rangle \langle i | H | j \rangle \langle j | k \rangle = H_{kk} = E_k \end{aligned} \quad (65)$$

where the relation $\langle i | H | j \rangle = \delta_{ij} \langle i | H | i \rangle$ is used for the exact eigenstates. The variance can be obtained using the matrix elements of H^2

$$\begin{aligned} \overline{(\Delta E)_k^2} &= \sum_i F_k^{(i)} \left(E_k - E^{(i)} \right)^2 \approx \sum_i \left| C_k^{(i)} \right|^2 \left(E_k - E^{(i)} \right)^2 \\ &= \sum_{p \neq k} H_{kp}^2 \end{aligned} \quad (66)$$

For example, in the two-body random interaction model with n particles distributed over m orbitals the sum in (66) can be evaluated exactly (see (56)).

Now, we calculate the first moment and variance of the energy spectrum. The trace conservation of H gives the first moment,

$$E_c = \frac{1}{N} \sum_k H_{kk} - \left(\frac{1}{N} \sum_k H_{kk} \right)^2$$

The conservation of $Tr H^2$ gives

$$\overline{E^2} = \frac{1}{N} \sum_k \langle k | H^2 | k \rangle = \frac{1}{N} \sum_{k,p} |H_{kp}|^2$$

which results in the relation

$$\begin{aligned} \sigma^2 \equiv \overline{E^2} - E_c^2 &= \frac{1}{N} \sum_{p,k} H_{pk} H_{kp} - E_c^2 \\ &= \frac{1}{N} \sum_k H_{kk}^2 + \frac{1}{N} \sum_{p \neq k} H_{pk}^2 - E_c^2 \\ &= \frac{1}{N} \sum_k E_k^2 - E_c^2 + \frac{1}{N} \sum_k \overline{(\Delta E)_k^2} = \sigma_0^2 + \overline{(\Delta E)^2} \end{aligned}$$

where σ_0^2 is the variance of the unperturbed spectrum and we have used Eq.(66).

Appendix 3. Calculations of spreading widths

To start with, we should stress that there are different definitions of the spreading widths. One of the natural definitions is $\Gamma_k \equiv 2\sqrt{\overline{(\Delta E)_k^2}}$ where $(\Delta E)_k^2$ is the variance of the distribution of the components $F_k^{(i)}$ (see (66)). In Ref. [3] it was shown that in the model of random two-body interaction this quantity is constant, $\Gamma_k = \Gamma$, see (56), i.e., it does not depend on a particular basis state (therefore, on excitation energy, number of excited particles n^* corresponding to this state, etc.). Note, it has a linear dependence on the interaction strength V .

Unlike the latter, the commonly used definition of the spreading width is related to the Breit-Wigner distribution and is defined as its half-width Γ_{BW} . However, this definition is reasonable only for relatively small interaction, when the form of the F -function is indeed close to

the Breit-Wigner form. In this case, the spreading width is given by the Fermi Golden Rule,

$$\Gamma_{BW}^{(k)} = 2\pi \frac{\overline{V_{kf}^2}}{d_f} \quad (67)$$

where d_f is the mean spacing between corresponding basis states $|f\rangle$ and V_{kf} is the matrix element of the interaction between the basis states $|k\rangle$ and $|f\rangle$ [24]. As one can see, the spreading width $\Gamma_{BW}^{(k)}$ is proportional to V^2 and differs from Γ . Note, that the second moment of the Breit-Wigner shape diverges, however, actual form has always cut-off in the tails which is reflected by the finite value of Γ .

If the interaction V is not small, the form of the F -function significantly differs from the Breit-Wigner shape (see Appendix 1). The critical value of V for this transition can be estimated from the condition $\Gamma_{BW}^{(k)} \approx \Gamma_k$.

Contrary to the spreading width Γ , the half-width of the Breit-Wigner shape depends on the basis state $|k\rangle$. Let us start with the estimate of the mean value of the spreading width $\Gamma_{BW}^{(k)}$. According to the definition (67), one needs to calculate the density of squared transition matrix elements $\overline{V_{kf}^2}/d_f = (\sum_f V_{kf}^2)/\Delta$ where the sum is taken over transitions from a given basis state $|k\rangle$ to other basis states $|f\rangle$ in the energy interval Δ . One should stress that the number of “allowed” transitions (due to the two-body interaction) is much less than the total number of basis states in this interval Δ . Let us assume, for simplicity, that the spacings d_0 between single-particle energy levels is constant and consider a pair of particles which occupy the orbitals s and q . If we move one particle to higher orbital and another particle to lower orbital by the same energy interval, the total energy of particles does not change. The total number of such moves is $M \approx (\min(m-s, q) + \min(m-q, s))/2$ where $m \gg 1$ is the number of orbitals. By averaging over all values s and q , one can obtain $M \approx m/3$. The Pauli principle reduces the number of available orbitals, therefore, in the system with n particles we have $M \approx (m-n)/3$. The number of possible pairs is given by $n(n-1)/2$, thus, the total number of basis states $|f\rangle$ which have the same energy and connected with the chosen basis state $|k\rangle$ is defined by

$$M_f \approx (m-n)n(n-1)/6 \quad (68)$$

Other basis states are separated by, at least, the energy distance d_0 . As a result, we obtain

$$\langle \Gamma_{BW} \rangle \approx 2\pi M_f \frac{V^2}{d_0} \approx \frac{\pi}{3} (m-n)n(n-1) \frac{V^2}{d_0} \quad (69)$$

It is interesting to note that the simple estimate involving total strength of transitions $(\Delta E)^2$, see Eq.(56), divided by the band-width $\Delta \sim d_0(m-n)$, gives close result. The above estimate (69) can be used when studying

the shape of the F -function in the regime of weak interaction. Note, the value of M_f defines the mean spacing between the “allowed” final states is

$$d_f = d_0/M_f \quad (70)$$

One should stress that the above estimate of M_f has been obtained for the spreading width averaged over all basis states. Near the ground state actual value of M_f is much smaller due to limitation of the available phase space. Also, the spreading width depends on the number of excited particles in the basis state. For example, one can calculate the spreading width Γ_{BW}^1 of the basis states with one excited particle only,

$$M_f = (s-n)^2; \quad \Gamma_{BW}^1 \approx \pi \frac{(s-n)^2 V_0^2}{d_0}; \quad s \leq 2n \quad (71)$$

$$M_f = n(2s-3n); \quad \Gamma_{BW}^1 \approx \pi \frac{n(2s-3n)V_0^2}{d_0}; \quad s > 2n \quad (72)$$

Here s is the position of a particle corresponding to the energy $\epsilon_s \approx s d_0$.

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FIGURE CAPTIONS

Fig.1. Analytical description of the occupation numbers. The data are given for the two-body random interaction model (1) of $n = 4$ Fermi-particles distributed over $m = 11$ orbitals with $V = 0.20$ and $d_0 = 1$ in the definition of single-particle energies, $\epsilon_s = d_0(s + \frac{1}{s})$, see [5,3,8]. The histogram is obtained according to (3) by the averaging over eigenstates with energies taken from small energy window centered at $E = 17.33$ and over 20 Hamiltonian matrices (1) with different realization of the random interaction. Stars represent the analytical expression (28) with σ_{0s} found from single-particle energy spectrum. Diamonds correspond to the Fermi-Dirac distribution with thermodynamical temperature (33) and chemical potential found from the standard condition for the total number of particles, $n = \sum_s n_s$.

Fig.2. Different temperatures versus the rescaled energy $\chi = (E - E_{fermi})/(E_c - E_{fermi})$ for the two-body random interaction model with $n = 4$ Fermi-particles and $m = 11$ orbitals. Triangles stand for the thermodynamical temperature T_{th} defined by (33) and should be compared to the canonical temperature T_{can} (circles), see (34). The width σ of the perturbed density of states is defined by the residual interaction $V = 0.12$ according to (18) and (56) with σ_0 found numerically from the unperturbed many-particle energy spectrum (the mean level spacing d_0 between single-particle levels is set to

$d_0 = 1$).

Fig.3. Fermi-Dirac distribution for strongly interacting particles. The data are given for the two-body random interaction model (1) with the parameters of Fig.1 (the rescaled energy is $\chi = 0.55$). Circles stand for the Fermi-Dirac distribution with the total energy E corresponding to the energy of eigenstates, see (23). Diamonds correspond to the shifted energy according to the expression (47).

Fig.4. Shift of the total energy for the corrected Fermi-Dirac distribution. The data are given for the model (1) with $n = 4, m = 11, d_0 = 1, V = 0.12$, see explanation in the text. The straight line is the analytical expression (47); the dotted line (circles) present direct computation of the shift based on the diagonalization of the Hamiltonian (1) with the following computation of the $\langle E_k \rangle_i$. On the horizontal axes the rescaled energy $\chi^{(i)} = (E^{(i)} - E_{fermi})/(E_c - E_{fermi})$ is plotted.

Fig.5. Distribution of the occupation numbers for small interaction. The histogram is obtained in the same way as in Figs.1-2, for the very weak interaction $V = 0.02$ which correspond to the region of (II) of the “initial chaoticization”, see Section 10. The total energy (center of the small energy window) is $E^{(i)} = 17.33$. Diamonds correspond to the theoretical expression (28) which is not valid in this region due to absence of equilibrium. Stars are obtained by direct numerical computation of n_s according to the F-distribution (5) with the F -function taken in the form (57), see Appendix 1 and [8]. The latter values are closer to the “experimental” ones since we performed summation over real unperturbed spectrum (instead of the integration with the Gaussian approximation for ρ_0 used to derive Eq. (28)).

Fig.1

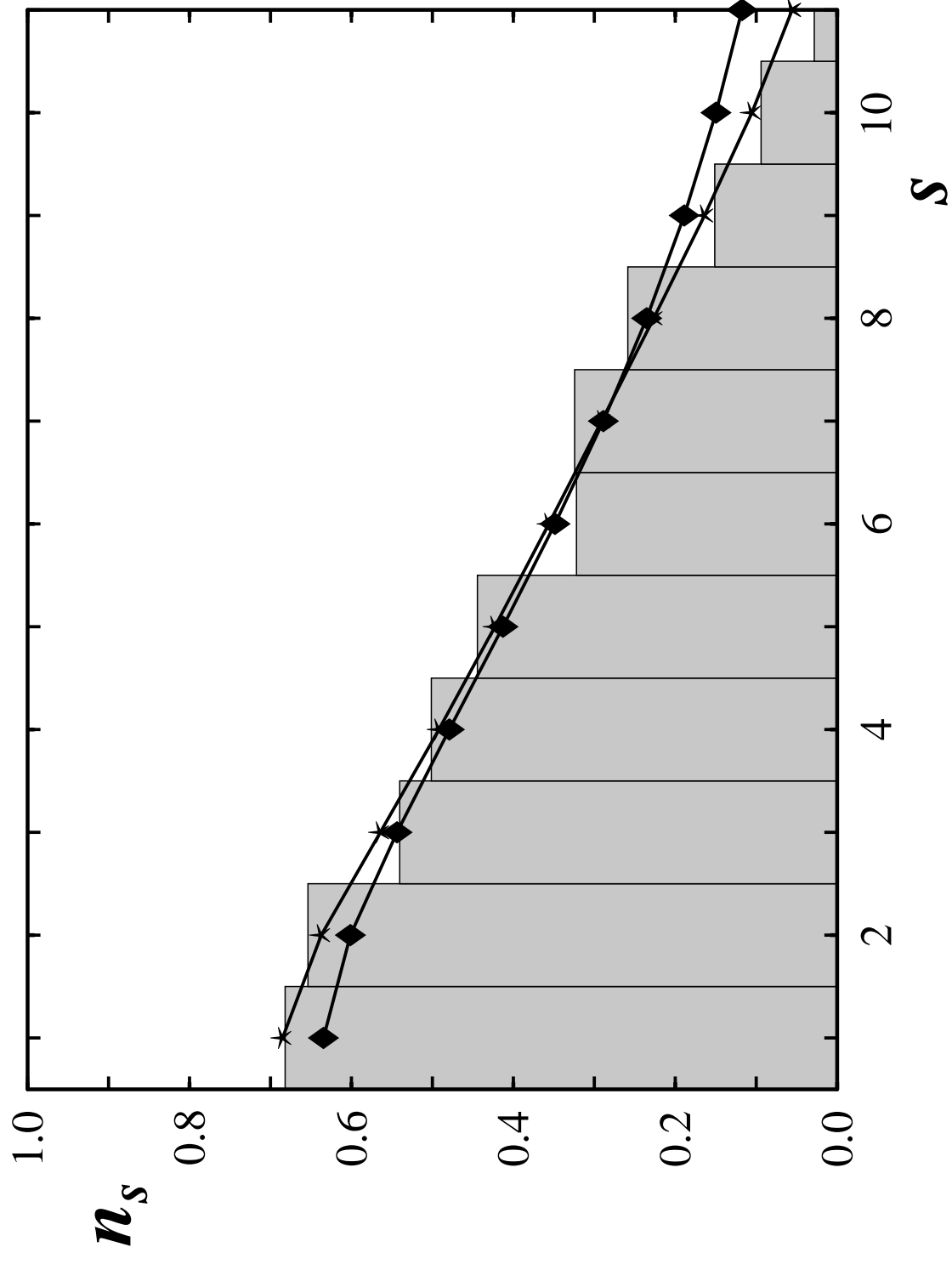


Fig.2

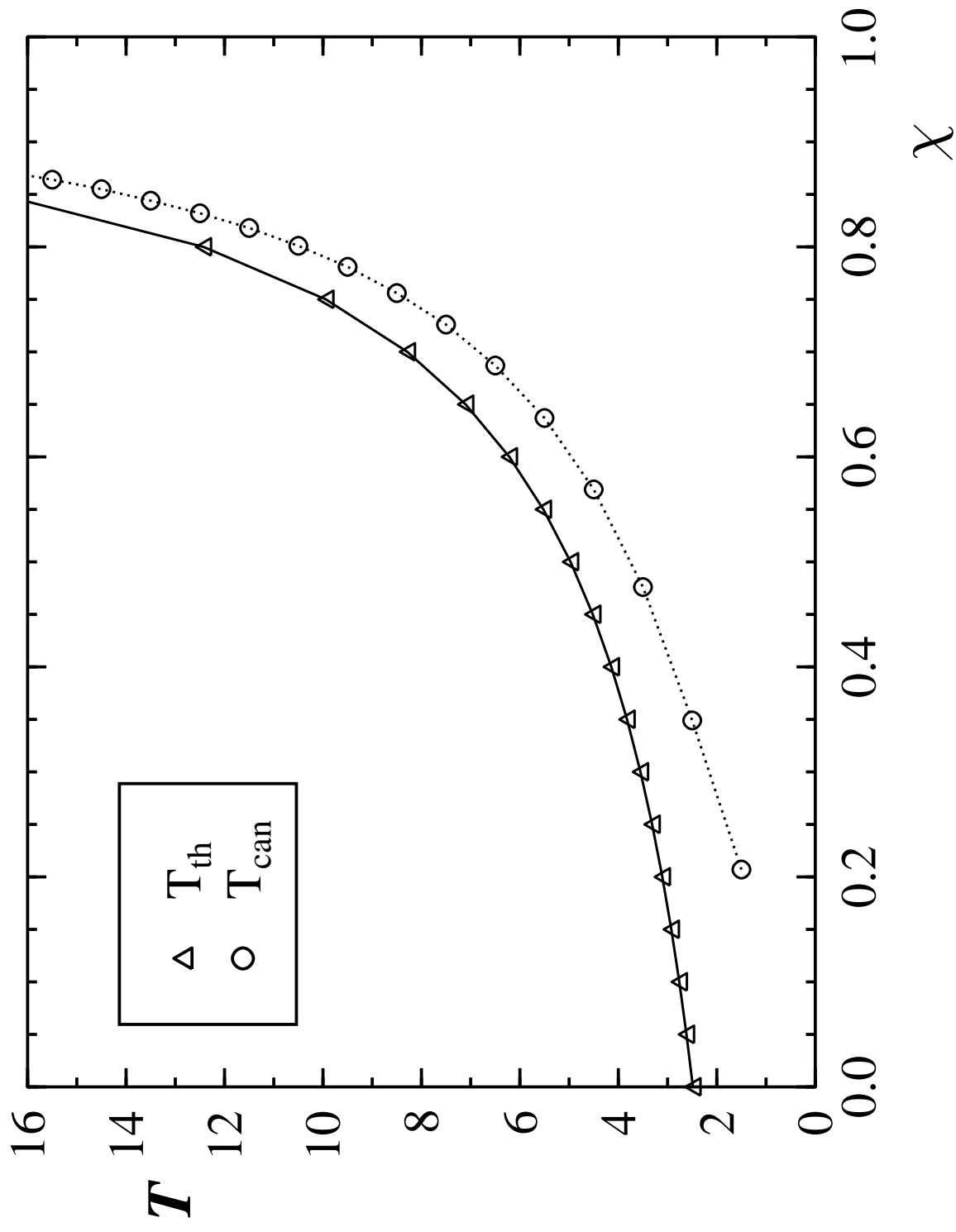


Fig.3

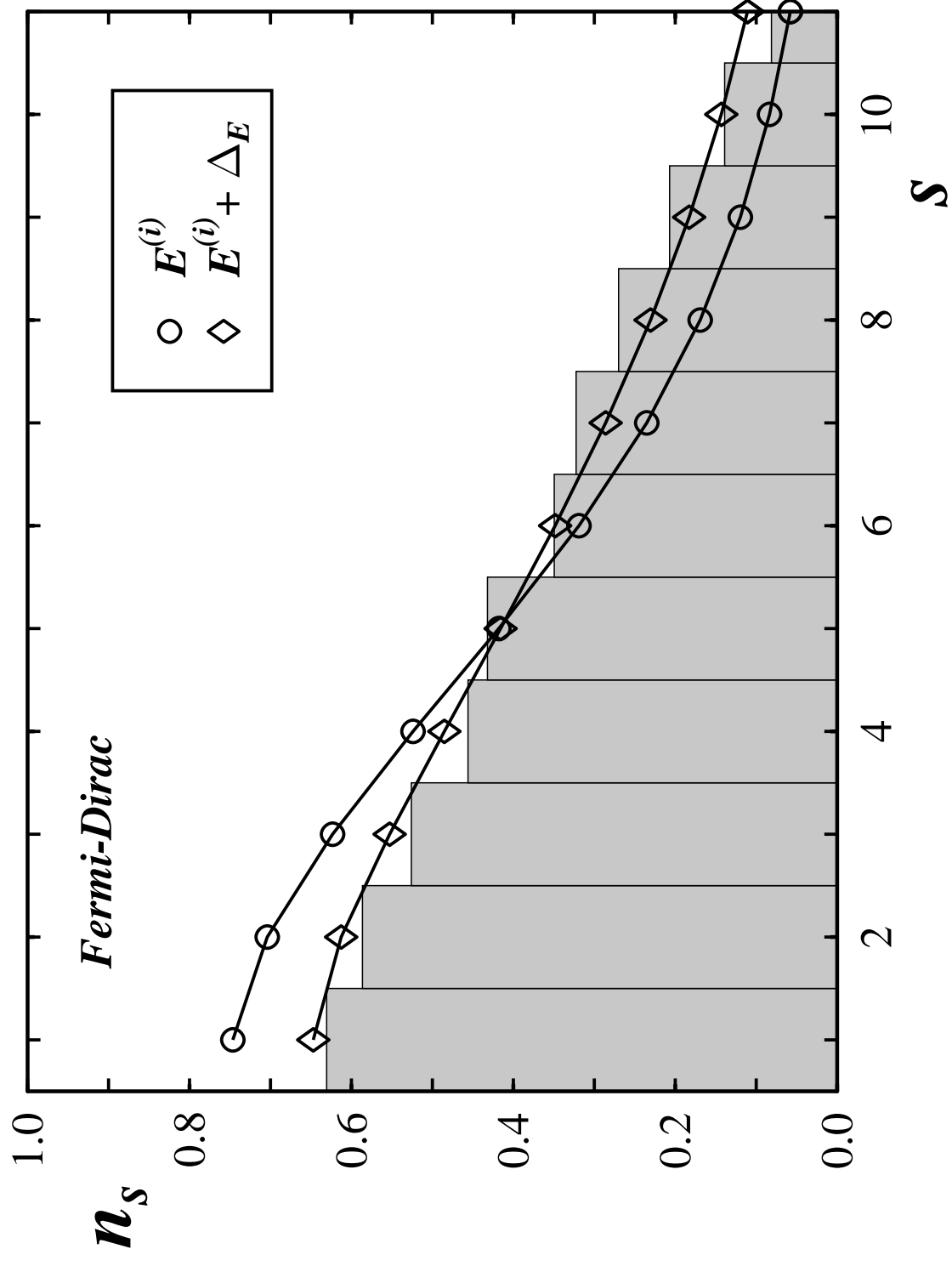


Fig.4

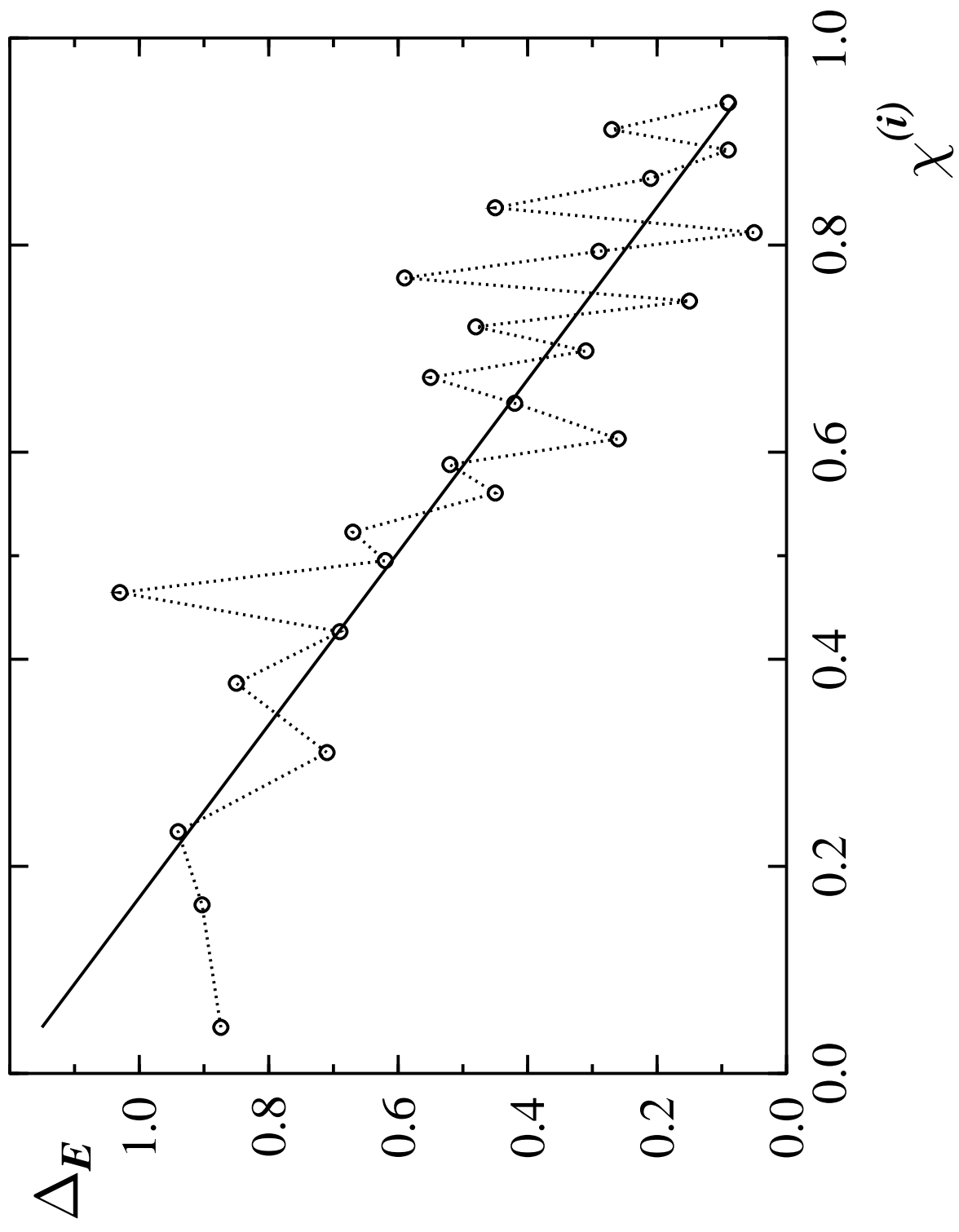


Fig.5

